# TECHNICAL NOTE

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# POSITRON-HYDROGEN SCATTERING

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## SUMMARY

The nonadiabatic theory of electron-hydrogen scattering is applied to the s-wave scattering of positrons by atomic hydrogen. This zeroth order problem is considerably more difficult than the corresponding one for electron-hydrogen scattering. If we assume that the most extensive of Rotenberg's calculation relating strictly to the zeroth order problem is an adequate approximation, then the present calculations support the conclusion that his final phase shifts are more correct than those of Schwartz. The nonadiabatic theory is also developed for higher partial wave scattering. The portion of the coupled set of equations which gives the major contribution to the phase shifts can readily be isolated. A first approximation of the truncated p-wave equations is obtained; the corresponding phase shifts are found to be positive, but much smaller than those of Bransden.

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## INTRODUCTION

The obtaining of reliable positron-hydrogen phase shifts has proven to be a very elusive task in spite of the fact that rigorous upper bounds exist for the scattering length (References 1 and 2) and in spite of the fact that in the latter reference as many as 50 variational parameters were used in obtaining the scattering length and phase shifts. The uncertainty in Schwartz's work has resulted from a recent calculation of Rotenberg (Reference 3) using a novel expansion in terms of Sturmian functions. His phase shifts are considerably larger than those of Schwartz. Further discussion of these differing results will be given later in this paper.

It should be noted, however, the conflicting results notwithstanding, that the phenomenological aspects of this problem are clear (sketched in Figure 1). At close distances the positron feels the repulsion of the positive nucleus and at far distances the attraction of the induced dipole moment of the hydrogen atom. These two extremes must be connected in some way. In Figure 1 the overall potential (solid curve) is taken to be the sum of the two dashed curves, one representing the repulsive Hartree potential

$$V_H = 2e^{-2r}\left(1 + r^{-1}\right)$$

and the other representing a phenomenological polarization potential

$$V_p = \frac{-\alpha}{\left(r^2 + d^2\right)^2} \quad ,$$

where $\alpha = 4.5\,d_0^3$ is the well-known polarizability of the hydrogen atom, and d is
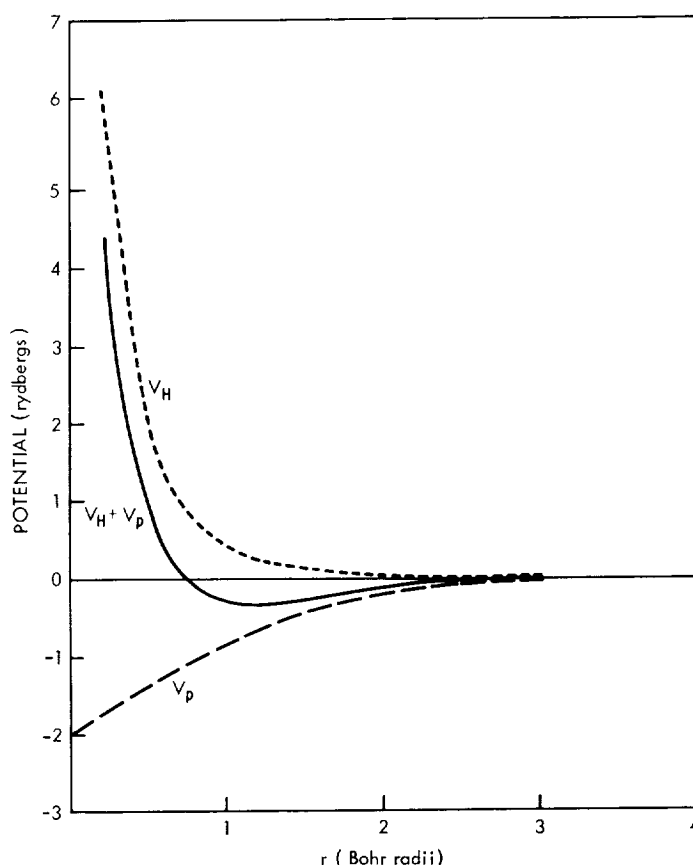


Figure 1—Phenomenological potentials describing the scattering of positrons from hydrogen.

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an adjustable parameter. In Table 1 we have given the phase shifts as a function of $k$ for two values of $d$, together with the phase shifts of Schwartz (Reference 2) and Rotenberg (Reference 3). At $k = 0.2$ we have included the result of the present calculation. The column for $d = \infty$ corresponds to the absence of polarization potential. The phase shifts of this static approximation have been computed before (Reference 4) and are negative in accord with the repulsive nature of Hartree potential. The next column, $d = 1.225$, has a special significance for the positron-hydrogen problem. The fact that these phase shifts are closer to and larger than Rotenberg's may be of significance.

Table 1

s-Wave Phase Shifts in Various Calculations.

| k (ryd $^{1/2}$) | Phase Shift (radians) | | | | |
|---|---|---|---|---|---|
| | $d = \infty$ | $d = 1.225$ | Reference 2 | Reference 3 | Nonadiabatic[†] |
| 0* | 0.58 | | − 2.10 | < − 2.7 | |
| 0.1 | − 0.0580 | 0.21 | 0.151 | 0.180 | |
| 0.2 | − 0.1145 | 0.29 | 0.188 | 0.232 | 0.22 |
| 0.3 | − 0.168 | 0.31 | 0.168 | 0.179 | |
| 0.4 | − 0.2181 | 0.29 | 0.120 | 0.129 | |
| 0.5 | − 0.2636 | 0.26 | 0.062 | 0.068 | |
| 0.6 | − 0.3043 | 0.23 | 0.007 | 0.010 | |
| 0.7 | − 0.340 | 0.19 | − 0.054 | − 0.04 | |

*The $k = 0$ entries are scattering lengths.
†Including relative s- and p-waves only.

The argument from which the value $d \approx 1.225$ is derived is surely very old (Reference 5). It is based on the observation that the potential which the positron sees (exclusive of its interaction with the nucleus) is identical to the energy of the electron in the combined field of the positron and the nucleus. However this energy is trivially calculable in the limit that the positron approaches the nucleus. In that case the electron sees simply a coulomb field of charge $Z = 2$. In other words we must have

$$\lim_{r \to 0} \left\{ \left[ 2e^{-2r}\left(1 + r^{-1}\right) - 2r^{-1} \right] - \frac{a}{\left(r^2 + d^2\right)^2} \right\} = -\frac{Z^2}{n^2} ,$$

where $n$ is the principal quantum member of the electron in its ground state (if we are dealing with the scattering by hydrogen in its ground state). Therefore using the value $n = 1$, $Z = 2$, and $a = 9/2$, the known polarizability of hydrogen, we can solve for $d$: $d = (9/4)^{1/4} \approx 1.225$.

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The remainder of this paper will be concerned with nonadiabatic theory of positron-hydrogen scattering. The quantitative results of this investigation are restricted to $k = 0.2$, since we are mainly concerned with establishing whether Schwartz's or Rotenberg's phase shifts are more correct. The calculations herein support the latter's results and, to that extent, agree with the phenomenological result previously stated.

## THE NONADIABATIC THEORY

The nonadiabatic theory starts with the decomposition of the s-wave function,*

$$\Psi\left(r_1, r_2, \theta_{12}\right) = \frac{1}{r_1 r_2}\sum_{l=0}^{\infty}(2l + 1)^{1/2}\Phi_l\left(r_1 r_2\right)P_l\left(\cos\theta_{12}\right),\tag{1}$$

which is complete in view of the fact that the Hamiltonian

$$H = -\frac{1}{r_1}\frac{\partial^2}{\partial r_1^2}r_1 - \frac{1}{r_2}\frac{\partial^2}{\partial r_2^2}r_2 - \left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}} + \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_{12}}$$

depends only upon the three coordinates $r_1$, $r_2$, $\theta_{12}$. As in electron-hydrogen problems these coordinates refer to the distance from the nucleus of the incoming particle(*positron* in this case) and the bound electron, and the angle between the respective radius vectors. One of the two salient differences between this and the electron-hydrogen problem is the changed signs of $2/r_1$ and $-2/r_{12}$ potentials. Here they are repulsive and attractive respectively. Thus the Hamiltonian is manifestly unsymmetrical with respect to $r_1$ and $r_2$, which implies that $\Psi\left(r_1, r_2, \theta_{12}\right)$ cannot be symmetrical—the second difference. Both these differences have profound consequences on the present problem as compared with the electron-hydrogen problem.

Substitution of Equation 1 into the Schrödinger equation

$$H\Psi = E\Psi\tag{2}$$

gives rise to the coupled set of equations

$$\left[\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} - l(l + 1)\left(r_1^{-2} + r_2^{-2}\right) + E + \frac{2}{r_2} - \frac{2}{r_1} + M_{ll}\right]\Phi_l = -\sum_{m(\neq l)}M_{lm}\Phi_m,\tag{3}$$

where

$$M_{lm} = \sqrt{(2l + 1)(2m + 1)}\sum_{n=0}^{l+m}\frac{r_<^n}{r_>^{n+1}}C_{lmn},$$

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*See Appendix A for list of symbols.

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with

$$C_{lmn} = \int_0^\pi P_l(\cos\theta)\, P_m(\cos\theta)\, P_n(\cos\theta)\, \sin\theta\, d\theta$$

the integral of three Legendre polynomials (Reference 7). The dependence of the $M_{lm}$ on $r_<^n/r_>^{n+1}$ means that there are two different equations depending on whether $r_1$ or $r_2$ is the larger. The equation for $\Phi_0$, for example, is more explicitly:

$$\left(\Lambda_{12} + E + \frac{2}{r_2}\right)\Phi_0^> = -\sum_{m=1}^\infty 2(2m+1)^{-1/2}\frac{r_2^m}{r_1^{m+1}}\Phi_m^> \quad,$$

$$\left(\Lambda_{12} + E - \frac{2}{r_1} + \frac{4}{r_2}\right)\Phi_0^< = -\sum_{m=1}^\infty 2(2m+1)^{-1/2}\frac{r_1^m}{r_2^{m+1}}\Phi_m^< \quad, \tag{4}$$

where

$$\Phi_l = \begin{cases} \Phi_l^< & r_1 < r_2 \\ \Phi_l^> & r_1 > r_2 \end{cases} \quad.$$

The boundary conditions are $\Phi_l(r_1\ 0) = 0 = \Phi_l(0,\ r_2)$ as long as we are below the threshold for inelastic scattering. Also, we have

$$\lim_{r_1 \to \infty} \Phi_l = \sin(kr_1 + \delta) R_{1s}(r_2)\, \delta_{l0}$$

and

$$\lim_{r_2 \to \infty} \Phi_l(r_1\ r_2) = 0 \quad.$$

The latter condition corresponds to the statement that below the inelastic threshold there are no states of a bound positron and a free electron; thus the wave function must vanish in the proper limit.

Since we have, in effect, two equations in two contiguous regions, appropriate matching conditions are required. Obviously they are

$$\Phi_l^< \Big|_{r_1=r_2} = \Phi_l^> \Big|_{r_1=r_2} \quad,$$

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and

$$\left[\frac{\partial}{\partial n} \Phi_i \right]_{r_1 = r_2} \qquad \left[\frac{\partial}{\partial n} \Phi_i \right]_{r_1 = r_2} \ . \tag{5}$$

The zeroth order problem is defined by neglecting the right side of Equation 4:

$$\left(\Lambda_{12} + E + \frac{2}{r_2}\right)\Phi_0^{(0)} = 0, \qquad\qquad r_1 > r_2 \tag{6a}$$

$$\left(\Delta_{12} + E - \frac{2}{r_1} + \frac{4}{r_2}\right)\Phi_0^{(0)} = 0. \qquad\qquad r_1 < r_2 \tag{6b}$$

The boundary conditions for $\Phi_0^{(0)}$ are in complete analogy to those for $\Phi_0$. In particular the zeroth order phase shift $\delta_0$ comes from the requirement that

$$\lim_{r_1 \to \infty} \Phi_0^{(0)} = \sin\left(k r_1 + \delta_0\right) R_{1s}\left(r_2\right) \ .$$

The zeroth order problem corresponds to a hydrogen atom and an incoming positron which sees no charge at all as long as it is outside the orbital electron, but which sees a repulsive (nuclear) potential when it is inside the electron. For this configuration the electron sees a doubly charged nucleus.

The basic relation between $\delta$ and $\delta_0$ is obtained by the usual procedure of pre-multiplication and integration of the $\Phi_0^{(0)}$ equation by $\Phi_0$ and vice-versa (see Reference 6). In this case the domain integration is shown in Figure 2. The area integrals involving $\Delta_{12}$ are converted to line integrals, and we use the diagonal boundary conditions (Equation 5) for $\Phi_0$ and the counterpart for $\Phi_0^{(0)}$,

$$\Phi_0^{(0)<}\Big|_{r_1 = r_2} = \Phi_0^{(0)>}\Big|_{r_1 = r_2} \ ,$$

$$\left[\frac{\partial}{\partial n} \Phi_0^{(0)<}\right]_{r_1 = r_2} = \left[\frac{\partial}{\partial n} \Phi_0^{(0)>}\right]_{r_1 = r_2} \ ,$$

to show that the line integrals along $s_3$ and $s_4$ cancel each other. The only
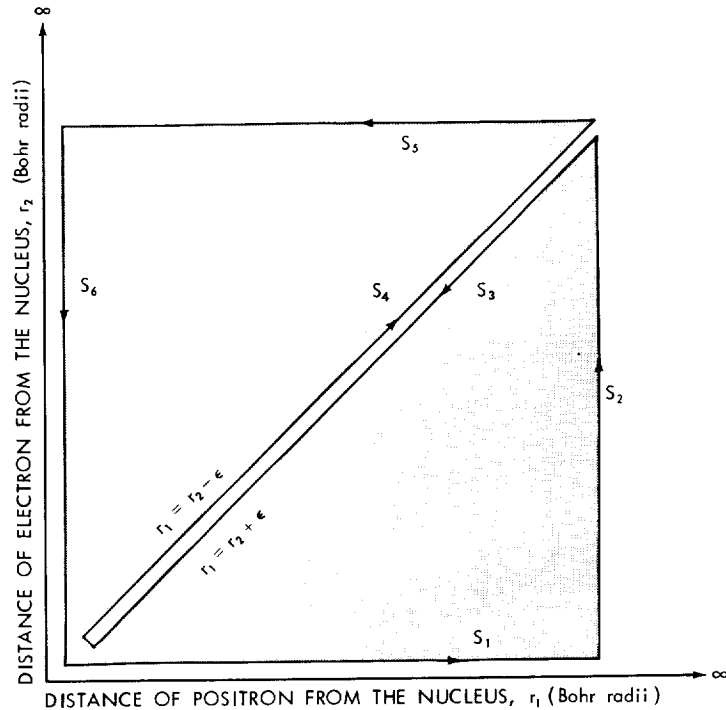


Figure 2—The domains of integration in obtaining the basic relation (Equation 7) for positron–hydrogen scattering.

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contribution comes from $s_2$, and we obtain

$$\sin\left(\delta - \delta_0\right) \approx k^{-1} \sum_{m=1}^{\infty} 2(2m+1)^{-1/2} \int_0^\infty \int_0^\infty dr_1\, dr_2\, \Phi_0^{(0)} \frac{r^m}{r^{m+1}} \Phi_m \quad . \tag{7}$$

## CALCULATIONS INVOLVING THE NONADIABATIC THEORY

From the verbal intepretation of the zeroth order problem we see clearly that it is a much cruder approximation of the complete positron-hydrogen scattering problem than the corresponding zeroth order problem for electron-hydrogen scattering. In particular it neglects the attraction of the positron to the electron and thus gives rise to negative phase shifts (for $\delta_0$), whereas the work of Spruch and Rosenberg (Reference 1) shows that the final $\delta$ must be positive as k approaches 0. The inadequacy in the description of the region $r_1 \approx r_2$ has a further consequence which can be demonstrated pictorially.

In Figure 3 we have sketched the probability of finding the electron at $r_1$ and the positron at $r_2$ as a function of $\theta_{12}$. As a result of the electron-positron attraction this probability must rise sharply for $\theta_{12} \approx 0$. Remembering that the basic decomposition (Equation 1) is in terms of Legendre polynomials, imagine that Figure 1 refers to an angular distribution curve for a differential scattering process. Such a process would be described as having large forward angle scattering, and this in turn would mean the contribution of many partial waves. In terms of the present formalism this corresponds to the contribution of many relative partial waves, and this means that Equation 2 cannot be expected to converge as rapidly as in the electron-hydrogen problem.

In the electron-hydrogen calculation, we also assumed, in addition to the assumption that there is a reasonably uniform convergence in $\Phi_l$ for increasing $l$, that the contribution from the configuration space $r_2 \approx r_1$ was small. The above discussion shows that the latter approximation is not justified. We shall therefore confine ourselves to solving the coupled set of equations;

$$\left(\Delta_{12} + E + \frac{2}{r_2} - \frac{2}{r_1} + \frac{2}{r}\right)\Phi_0 = -\frac{2}{\sqrt{3}}\frac{r_<}{r_>^2} \Phi_1 \quad , \tag{8a}$$

$$\left(\Delta_{12} + E + 2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\right.$$

$$\left. + \frac{2}{r_2} - \frac{2}{r_1} + \frac{2}{r_>} + \frac{4}{5}\frac{r_<^2}{r_>^3}\right)\Phi_1 = -\frac{2}{\sqrt{3}}\frac{r_<}{r_>^2} \Phi_0 \quad , \tag{8b}$$



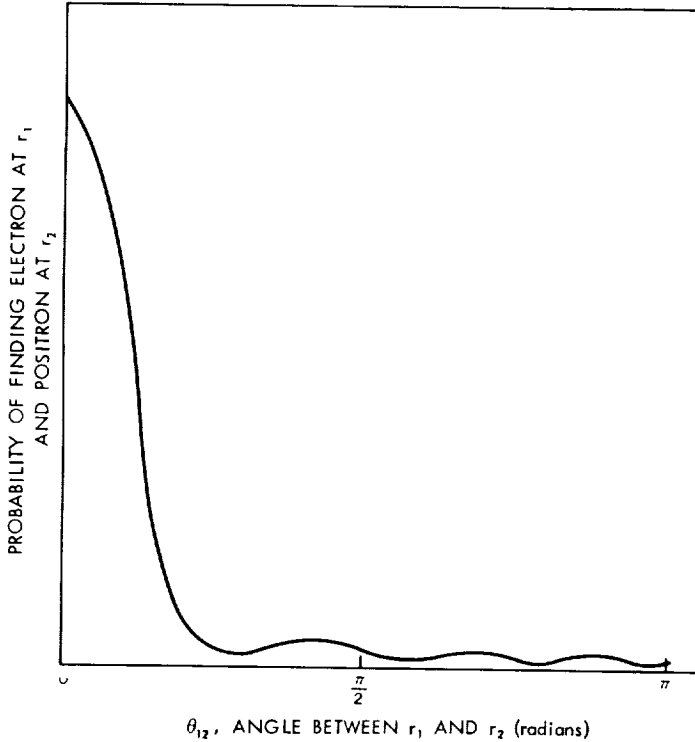$\theta_{12}$, ANGLE BETWEEN $r_1$ AND $r_2$ (radians)

Figure 3—The probability of finding a positron and a hydrogenic electron at distances $r_1$ and $r_2$ from the origin as a function of the angle between the radii and vectors.

which were obtained by truncating Equation 3 beyond $\Phi_1$ but without making any assumption about $r_<^n / r_>^{n+1}$.

First it is necessary to solve the zeroth order problem defined by Equation 6 and the boundary conditions. Assuming that $\Phi_0^{(0)}$ is known, we can consider a first approximation of $\Phi_1$ as the solution of

$$\left( \Delta_{12} - 2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) + E + \frac{2}{r_2} - \frac{2}{r_1} + \frac{2}{r_>} + .8 \frac{r_<^2}{r_>^3} \right) \Phi_1^{(0)} = \frac{-2}{\sqrt{3}} \frac{r_<}{r_>^2} \Phi_0^{(0)} . \tag{9}$$

The following sum rules are useful in the subsequent development:

$$\int_0^\infty \int \Phi_0^{(0)} \left[ -2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) + .8 \frac{r_<^2}{r_>^3} \right] \Phi_1^{(0)} \, dr_1 \, dr_2 = \frac{2}{\sqrt{3}} \int_0^\infty \int \frac{r_<}{r_>^2} \left(\Phi_0^{(0)}\right)^2 dr_1 \, dr_2 , \tag{10a}$$

$$\int_0^\infty \int \Phi_0 \left[ -2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) + .8 \frac{r_<^2}{r_>^3} \right] \Phi_1 \, dr_1 \, dr_2 = \frac{2}{\sqrt{3}} \int_0^\infty \int \frac{r_<}{r_>^2} \left[ (\Phi_0)^2 - (\Phi_1)^2 \right] dr_1 \, dr_2 . \tag{10b}$$

From Equations 8b and 9 we can also derive

$$\int_0^\infty \int \left( \Phi_1^{(0)} \Phi_0 - \Phi_1 \Phi_0^{(0)} \right) \frac{r_<}{r_>^2} \, dr_1 \, dr_2 = 0 . \tag{11}$$

We can write

$$\Phi_1 = \Phi_1^{(0)} + \Delta\Phi_1 ,$$

$$\Phi_0 = \Phi_0^{(0)} + \Delta\Phi_0 ;$$

Equation 11 now implies

$$\int_0^\infty \int \frac{r_<}{r_>^2} \Phi_1^{(0)} \Delta\Phi_0 \, dr_1 \, dr_2 = \int_0^\infty \int \frac{r_<}{r_>^2} \Phi_0^{(0)} \Delta\Phi_1 \, dr_1 \, dr_2 . \tag{12}$$

A sufficient condition for the satisfaction of Equation 12 is

$$\Phi_1^{(0)} \Delta\Phi_0 = \Phi_0^{(0)} \Delta\Phi_1 .$$

This equality is almost certainly too strong to be exactly true, but it is difficult to see why it should not be satisfactory as an approximation. Further, writing

$$\Delta\Phi_1 = C \Phi_1^{(0)} g\left(r_1, r_2\right) , \tag{13}$$

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we can put Equation 10b into the form:

$$2C \int_0^\infty \int \Phi_0^{(0)} \left[ 2\left(\frac{1}{r_1^2} + \frac{1}{r_2}\right) - .8 \frac{r_2^2}{r_3} \right] \Phi_1^{(0)} \, g(r_1 r_2) \, dr_1 \, dr_2$$

$$+ C^2 \int_0^\infty \int \Phi_0^{(0)} \left[ 2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) - .8 \frac{r_2^2}{r_3} \right] \Phi_1^{(0)} \left[ g(r_1 r_2) \right]^2 dr_1 \, dr_2$$

$$- \frac{2}{\sqrt{3}} \int_0^\infty \int \frac{r_2}{r^2} (\Phi_1^{(0)})^2 \, dr_1 \, dr_2 + \frac{4C}{\sqrt{3}} \int_0^\infty \int \frac{r_2}{r^2} \left[ (\Phi_0^{(0)})^2 - (\Phi_1^{(0)})^2 \right] g(r_1 \, r_2) \, dr_1 \, dr_2$$

$$+ 2(3)^{-1/2} C^2 \int\int \frac{r_2}{r^2} \left[ (\Phi_0^{(0)})^2 - (\Phi_1^{(0)})^2 \right] \left[ g(r_1 \, r_2) \right]^2 dr_1 \, dr_2 \quad . \tag{14}$$

In writing $\Delta\Phi$ in the form of Equation 13 we consider $g(r_1 r_2)$ a fixed function, and $C$ a constant determined by the solution of the quadratic equation (Equation 14). We have chosen

$$g(r_1 \, r_2) = \left(\frac{r_2}{r_1}\right) \exp\left(-\frac{r_2}{r_1}\right) \quad . \tag{15}$$

This function vanishes at $r_1 = 0$, $r_2 = 0$; is continuous with continuous derivative across $r_1 = r_2$; and has a maximum at $r_1 = r_2$.

In order to evaluate the integrals in Equation 14, it is also necessary to know $\Phi_1^{(0)}$. This can be handled just as in the electron-hydrogen problem (Reference 6), viz., we append a parameter $D$ to the adiabatic form of $\Phi_1^{(0)}$:

$$\Phi_1^{(0)} = \frac{2}{\sqrt{3}} \frac{\sin(kr_1 + \delta_0)}{r_1^2 + D} e^{-r_2} \left(\frac{r_2^3}{2} + r_2^2\right) \quad ,$$

where $D$ is determined such that Equation 8a is satisfied. Thus we are left with the difficult problem of evaluating $\Phi_0^{(0)}$. The expansion used in the electron-hydrogen case simply will not work here. In the region $r_1 < r_2$ there is only one separable solution of Equation 6b; in addition, it is difficult to formulate a useful expression which will minimize the deviation from both boundary conditions simultaneously (Equation 5).

It should be noted, however, that as in the electron-hydrogen problem (Reference 6) any attack on the complete problem with functions of $r_1$ and $r_2$ can only approximate the zeroth order problem. At least three approximations have been carried out which fall into this category. One is the static approximation, the second an (unsymmetrical) close-coupling approximation with 1s-2s-3s hydrogenic states included (Reference 4), and the third that part of Rotenberg's calculation (Reference 3) in which no $\vartheta_{12}$ dependence is contained. It was originally thought that the static approximation would be sufficient for quantitative purposes. The supposition seemed to be confirmed by the fact that the inclusion of the 2s and 3s states (Reference 4) increased the static phase shifts by less than 4 percent.

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Therefore, in the first instance we used the 1s-2s-3s approximation for $\Phi_0^{(0)}$:

$$\Phi_0^{(0)} = \sum_{n=1}^{3} u_n (r_1) R_{ns} (r_2) .$$

(16)

The integrals in the above development could then be evaluated. In order to satisfy the dipole sum rule (Equation 10a) we found it necessary to augment $\Phi_1^{(0)}$. Let $\tilde{\gamma}$ be the phase shift of the problem defined by the coupled set (Equation 8). The, according to the above development,

$$\sin\left(\tilde{\gamma} - \delta_0\right) = \frac{2}{k\sqrt{3}} \int_0^\infty \int \Phi_0^{(0)} \frac{r_<}{r_>^2} \Phi_1^{(0)} dr_1 dr_2 + \frac{2}{k\sqrt{3}} \int_0^\infty \int \Phi_0^{(0)} \frac{r_2}{r_>^2} C\Phi_1^{(0)} g\, dr_1 dr_2 .$$

(17)

At $k = 0.2$ we obtained the values 0.1414 and 0.0042 for the two terms on the right side of Equation 17. With $\delta_0 = -0.1102$ as given by the above $\Phi_0^{(0)}$, we obtained

$$\tilde{\gamma} = \delta_0 + \sin^{-1}(0.1456) = 0.0359 .$$

The value of $\delta$ obtained by Spruch and Rosenberg (Reference 1) at $k = 0.2$ is 0.150. This value can be taken as a reliable (but not rigorous) lower bound on the phase shift. As mentioned previously, the multipole expansion cannot be expected to converge as dramatically as in the electron-hydrogen case; nevertheless the difference between these two numbers seemed greater than could be attributed to higher multipoles.

To check this, we computed several terms of Equation 7 using the appropriate projections of the Spruch-Rosenberg wave function (Reference 1) to obtain $\Phi_l$ and using Equation 16 for $\Phi_0^{(0)}$. The results for $k = 0.2$ are given in Table 2. The last row is obtained from Equation 7 using the first three terms and the appropriate value of $\delta_0$ (in the $l = 0$ row). This $\delta$ is reasonably close to 0.150 which Spruch and Rotenberg obtained from their complete calculation. The results indicate that the contribution of the higher multipoles is fairly small—although not negligible—and that the main discrepancy is in the dipole contribution: 0.194 versus our 0.146. There could be many causes for this discrepancy and for the apparent consistency of the Spruch-Rosenberg wave function with the Smith-Burke $\Phi_0^{(0)}$. As far as the present calculation was concerned, it was felt after much delibration that the approximation (Equation 16) for $\Phi_0^{(0)}$ must somehow be inadequate.

This supposition has very recently been markedly supported by the work of Rotenberg (Reference 3). Insofar as it bears on the zeroth order problem, his expansion is of the form of Equation 16 with the hydrogenic functions $R_{ns} (r_2)$ replaced by the Sturmian functions $S_{n0}(r_2)$ . In this approximation

$$\Phi_0^{(0)} = \sum_{n=1}^{3} u_n (r_1) S_{n0} (r_2) .$$

(18)

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## Table 2

Results of Spruch-Rosenberg
Wave Function for $k = 0.2$.

| $l$ (radians) | Multipole Integral |
|---|---|
| 0 | $-0.1102$ |
| 1 | $0.194$ |
| 2 | $0.0377$ |
| 3 | $0.00947$ |
| $\delta$ | $0.131$ |

$S_{10}(r_2)$ is identical to $R_{1s}$, and the remaining Sturmian functions (with our normalization) are:

$$S_{20}(r) \quad 2\sqrt{2}\, e^{-r}\left(r - r^2\right) ,$$

$$S_{30}(r) \quad 2(3)^{-1/2}\, e^{-r}\left(3r - 6r^2 + 2r^3\right) .$$

The chief property of the Sturmian function is that they are a complete set without a continuous spectrum (Reference 3). The effect of this expansion on the zeroth order phase shift can be gleaned from the first three columns of row b, Table 3 (taken from Table II of Reference 3) for $k = 0.2$. The first three columns refer to the zeroth order

## Table 3

Effect of Adding Terms.

| Type of Function | Total Number of Terms* | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Sturmian (row b) | $-0.067$ | $-0.041$ | $-0.022$ | $0.057$ | $0.093$ | $0.195$ | $0.212$ | $0.232$ |
| Hydrogenic (row c) | $-0.1145$ | $-0.1109$ | $-0.1102$ | $-$ | $-$ | $-$ | $-$ | $-$ |

*Taken successively as $(n, L) = (1, 0), (2, 0), (3, 0), (2, 1), (3, 1), (4, 1), (3, 2), (4, 2)$.

problem, and are to be compared to successive augmentation of the hydrogenic wave functions 1s, 2s, 3s in the close coupling expansion row c (Reference 4). Then, according to Rotenberg's results, the convergence of the close-coupling expansion is spurious, and the correct zeroth order phase shift is much less negative than had hitherto been thought.* Using Equation 18 for $\Phi_0^{(0)}$, we obtain from the nonadiabatic theory, as outlined above, the contributions 0.227 and 0.0169 for the two terms of Equation 17. This in turn yields a $\tilde{\delta} = 0.224$.

The calculation was repeated using the Ansatz

$$\Phi_1^{(0)} \quad - \quad \frac{2}{\sqrt{3}} \frac{u_1(r_1)}{r_1^2 + D} e^{-r_2}\left(\frac{r_2^3}{2} + r_2^2\right) ,$$

where $u_1(r_1)$ is first function in Equation 18. In this case we obtained the values .222 and .0172 and a final $\tilde{\delta} = 0.219$. These results agree to two figures and are compared with the entry in column 6

*Nevertheless, as long as the phase shifts are negative, we can find a physical rationalization for the result; the part of the positron's wave function inside the orbital electron makes the latter see effectively a more positively charged nucleus. This makes the electron more tightly bound; thus the part of the positron's wave function outside of the electron sees a repulsive but much smaller structure, giving rise to negative but smaller (in absolute value) phase shifts. It is evident that such a picture corresponds to a highly nonadiabatic situation.

($\tilde{\gamma}$ = 0.195) of Table 3. Up to this point only relative s- and p-states have been included; so that, through column 6, Rotenberg approximates the solution of the coupled set (Equations 8). The comparison shows that with the inclusion of three $(n, l)$ terms he has almost obtained convergence, relative to having $\Phi_0$ described by three $(n, 0)$ terms. The subsequent addition of d-wave terms gives an additional contribution 0.037 to his phase shift. This agrees identically to the $l = 2$ contribution (Table 2) of the Spruch-Rosenberg wave function. The exact agreement is undoubtedly coincidental, but it adds confidence that this contribution, too, is well represented by the Sturmian expansion.

It follows that, if the Sturmian expansion (Equation 18) for $\Phi_0^{(0)}$ is essentially correct, then Rotenberg's phase shifts are more correct than those of Schwartz (Reference 2; see also Table 1) and that the former are very likely a lower bound.

Two questions immediately present themselves. First, how adequate is the Sturmian expansion of $\Phi_0^{(0)}$? The lack of convergence of Rotenberg's results is most noticeable in his zeroth order results. Indeed, naively extrapolating the first three columns of Table 3 might lead to a positive zeroth order phase shift—a conclusion which, in view of the physical interpretation of the zeroth order problem, is almost inconceivable. We suspect that the convergence of the Sturmian expansion is exceedingly rapid, so that within the addition of the first couple of terms the phase shift rapidly approaches the converged value and that the change, after a couple of terms have been added, is very small. If this is the case, then we must sincerely applaud this remarkable expansion. For the present, however, the possibility cannot be excluded that the inclusion of more $(n, 0)$ Sturmian functions will make the phase shift retreat towards the close-coupling value.

The second question is, if Rotenberg's results (Reference 3) are basically correct, how can Schwartz's results (with many parameters) be so incorrect? This is a difficult question to answer. However, it should be noted that the number of terms in his wave function relating exclusively to the zeroth order problem is not overly great. Therefore his calculation may be inadequate precisely because it does not describe sufficiently the correlations of the zeroth order problem. If this is the case, it provides an additional reason for considering the zeroth order problem separately from the remainder of the scattering problem—which is the essence of the nonadiabatic theory.

In the recent work of Reference 8, an adiabatic polarization potential $\alpha(r)/r^4$, where

$$\alpha(r) = \frac{9}{2} - e^{-2r}\left(\frac{2r^5}{3} + 3r^4 + 6r^3 + 9r^2 + 9r + \frac{9}{2}\right),$$

is used in place of the phenomenological potential $\alpha/(r^2 + d^2)^2$. The latter was derived (Reference 9)* specifically for the problem of *electron-hydrogen* scattering (Reference 10) as a prototype of *electron-atom* scattering (Reference 11). In that case it was shown (Reference 6) that, beyond the spherically symmetric zeroth-order approximation, the phase shift is dominated by the dipole correction. Now the

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*The potential $\alpha(r)/r^4$ was derived by multiplying the adiabatic dipole term in the wave function by a step function. This function has a discontinuity in value and an infinite discontinuity in slope at $r_1 = r_2$. Both these features are removed in the $e^-$-H problem by (anti) symmetrizing the total wave function. However, in the $e^+$-H problem, the ansatz for the wave function retains these unpleasant features, since there is no symmetrization.

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$\alpha(r)/r^4$ potential goes to zero at $r = 0$ whereas the $\alpha/(r^2 + d^2)^2$ potential does not (see Figure 1). Thus the effect of the attraction in the former is suppressed for small $r$ and phenomenologically simulates the contribution of only the dipole ($l = 1$) term in the nonadiabatic description. However, from Table 2 it is clear that in positron-hydrogen scattering a significant contribution comes from the higher relative partial waves. The stronger dependence of the $\alpha/(r^2 + d^2)^2$ potential near the origin appears better suited to simulate this contribution.

## NONADIABATIC THEORY OF HIGHER PARTIAL WAVE SCATTERING

Let $\psi_L$ be the wave function of the partial wave of angular momentum $L$. For the elastic scattering problem,

$$\lim_{r_1 \to \infty} \psi_L = \frac{\sin\left(kr_1 - \frac{1}{2}\pi l + \delta^{(L)}\right)}{r_1} Y_{L_0}(\Omega_1) \frac{R_{1s}(r_2)}{r_2} Y_{00}(\Omega_2) .$$

We can expand this wave function

$$\psi_L = \frac{1}{r_1 r_2} \sum_{l_1, l_2} \Phi_{l_1 l_2}^{(L)}(r_1 r_2) \sum_{m_1} \left(l_1 l_2 m_1 - m_1 \mid L0\right) Y_{l_1 m_1}(\Omega_1) Y_{l_2 -m_1}(\Omega_2) , \tag{19}$$

where $\left(l_1 l_2 m_1 m_2 \mid LM\right)$ are the Clebsh-Gordon coefficients in the notation of Condon and Shortley (Reference 7). With this expansion the Schrödinger equation can be reduced to

$$\left[ \nabla_{12} - \frac{l_1(l_1 + 1)}{r_1^2} - \frac{l_2(l_2 + 1)}{r_2^2} - \frac{2}{r_1} + \frac{2}{r_2} \right.$$

$$\left. + E + \left\langle l_1 l_2 \left| \frac{2}{r_{12}} \right| l_1 l_2 \right\rangle \right] \Phi_{l_1 l_2}^{(L)} = -\sum_{\lambda_1, \lambda_2}' \left\langle l_1 l_2 \left| \frac{2}{r_{12}} \right| \lambda_1 \lambda_2 \right\rangle \Phi_{\lambda_1 \lambda_2}^{(L)} , \tag{20}$$

where

$$\left\langle l_1 l_2 \left| \frac{2}{r_{12}} \right| \lambda_1 \lambda_2 \right\rangle = \sum_{m_1} \left(l_1 l_2 m_1 - m_1 \mid L0\right)^2 \iint Y_{l_1 m_1}^*(\Omega_1) Y_{l_2 -m_1}^*(\Omega_2) \frac{2}{r_{12}} Y_{\lambda_1 m_1}(\Omega_1) Y_{\lambda_2 -m_1}(\Omega_2) d\Omega_1 d\Omega_2 .$$

The quantities $l_1$, $l_2$, and L must satisfy the usual triangular equality. In addition $l_1 + l_2$ and L must have the same parity. From Equation 20 it is clear that the effective centrifugal barrier which a given $\Phi_{l_1 l_2}^{(L)}$ sees is determined by $l_1 + l_2$. For a given L (L $\neq$ 0) there are two functions which are associated with the lowest centifugal barrier $\left(l_1 + l_2 = L\right)$, $\Phi_{L0}^{(L)}$ and $\Phi_{0L}^{(L)}$. The rule of parity then says that the next functions which enter the expansion (Equation 19) must have a centrifugal barrier *two* units greater than L. Thus we have a powerful argument that the higher partial wave scattering is determined mainly by the coupled set of equations for the lowest two functions.

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Applying this approximation to p-wave scattering (and suppressing the superscript 1), we get:

$$\left(\Delta_{12} - \frac{2}{r_1^2} - \frac{2}{r_1} + \frac{2}{r_2} + \frac{2}{r_>} + E\right)\Phi_{10} = -\left(\frac{2}{3}\right)\left(\frac{r_<}{r_>^2}\right)\Phi_{01} \, ,$$

$$\left(\Delta_{12} - \frac{2}{r_2^2} - \frac{2}{r_1} + \frac{2}{r_2} + \frac{2}{r_>} + E\right)\Phi_{01} = -\left(\frac{2}{3}\right)\left(\frac{r_<}{r_>^2}\right)\Phi_{10} \qquad (21)$$

where the boundary conditions are

$$\lim_{r_1 \to \infty} \Phi_{10} = \sin\left(kr_1 + \gamma^{(L)} - \frac{\pi}{2}\right) R_{1s}\left(r_2\right) \, ,$$

$$\lim_{r_1 \to \infty} \Phi_{01} = 0 \, , \qquad (22)$$

plus the vanishing of these functions in all other asymptotic regions.

Now since both $\Phi_{10}$ and $\Phi_{01}$ are associated with the same amount of centifugal barrier, we expect a reliable solution will be reasonably simultaneous. As a very first approximation, however, we may note that there is a great asymmetry in the boundary conditions, Equation 22, and between $\Phi_{10}$ and $\Phi_{01}$, leading to the qualitative expectation that the former function is dominant over the latter. Within this approximation we could consider a zeroth order problem:

$$\left(\Delta_{12} - \frac{2}{r_1^2} - \frac{2}{r_1} + \frac{2}{r_2} + \frac{2}{r_>} + E\right)\overset{0}{\Phi}_{10} = 0 \, , \qquad (23)$$

with the asymptotic solution

$$\lim_{r_1 \to \infty} \overset{0}{\Phi}_{10} = \sin\left(kr_1 - \frac{\pi}{2} + \delta_0^{(1)}\right) R_{1s}(r_2) \, .$$

We can then readily derive

$$\sin\left(\gamma^{(1)} - \delta_0^{(1)}\right) = \frac{2}{3k} \int_0^\infty \int_0^\infty \overset{0}{\Phi}_{10} \frac{r_<}{r_>^2} \Phi_{01} \, dr_1 \, dr_2 \, . \qquad (24)$$

from Equations 21 and 23. Equation 24 is exact; the approximation comes in when we replace $\Phi_{01}$ by the approximation $\overset{0}{\Phi}_{01}$, which is governed by

$$\left(\Delta_{12} - \frac{2}{r_2^2} - \frac{2}{r_1} + \frac{2}{r_2} + \frac{2}{r_>} + E\right)\overset{0}{\Phi}_{01} = -\frac{2}{3}\frac{r_<}{r_>^2}\overset{0}{\Phi}_{10} \, .$$

From this equation and Equation 23, we obtain

$$\int_0^\infty \int \overset{0}{\Phi}_{10} \left( \frac{2}{r_2^2} - \frac{2}{r_1^2} \right) \overset{0}{\Phi}_{01} \, dr_2 \, dr_2 \; = \; \frac{2}{3} \int_0^\infty \int \left( \overset{0}{\Phi}_{10} \right)^2 \frac{r_<}{r_>^2} \, dr_1 \, dr_2 \; .$$

(25)

The following approximations are used in solving for $\overset{\sim}{\delta}{}^{(1)}$:

$$\overset{0}{\Phi}_{10} \; = \; kr_1 \, j_1 (kr_1) \; ,$$

where $j_1(kr)$ is the spherical Bessel function and, by implication, $\delta_0^{(1)} = 0$; and

$$\overset{0}{\Phi}_{01} \; = \; \frac{2}{3} \frac{kr_1 \, j_1 (kr_1)}{r_1^2 + D} \, e^{-r_2} \left( \frac{r_2^3}{2} + r_2^2 \right) \; ,$$

which is the adiabatic form of $\Phi_{01}$. In principal D is to be determined by the satisfaction of Equation 25. Actually we were unable to satisfy the sum rule with $\overset{0}{\Phi}_{01}$ in the above form. Therefore we had to change $\overset{0}{\Phi}_{01}$ to $\overset{\sim}{\Phi}_{01}$:

$$\overset{\sim}{\Phi}_{01} \; = \; \overset{0}{\Phi}_{01} \left( 1 + Cg(r_1 r_2) \right) \; ,$$

where $g(r_1 r_2)$ is given in Equation 15, D was chosen as unity, and C was varied to give equality. We can now determine $\overset{\sim}{\delta}{}^{(1)}$ by using

$$\overset{\sim}{\delta}{}^{(1)} \; \approx \; \frac{2}{3k} \int_0^\infty \int \overset{0}{\Phi}_{10} \frac{r_<}{r_>^2} \overset{\sim}{\Phi}_{01} \, dr_1 \, dr_2 \; .$$

In obtaining these results we have thus made two approximations. The first is the replacement of the exact p-wave equation by the truncated set (Equation 21), which is equivalent to neglecting the difference between $\delta^{(1)}$ and $\overset{\sim}{\delta}{}^{(1)}$. We would expect that this would not introduce an error of more than 25 percent—erring on the small side. We have also approximated the solution of Equation 21. However, in this case $\delta_0^{(1)}$ is an over-estimate of the exact $\delta_0^{(1)}$, which must surely be negative. On the whole therefore the final phase shifts in Table 4 can reasonably be expected to be within a factor 2 of the exact p-wave phase shifts. The discrepancy with Bransden's phase shifts (Reference 12, and also Table 4) is generally greater than this amount.

The phase shifts are essentially negligible as far as the total cross section is concerned. The s-wave cross sections are presented in Figure 4. It can be seen that it will be very difficult to distinguish experimentally between the results of Schwartz and Rotenberg. (There is a remote possibility at 0.5 ev.) On the other hand, in the region of the minimum (5 ev) the p-wave will yield a cross section of less than 0.5 $\pi a_0^2$ whereas, according to Bransden, the cross section should be about $\pi a_0^2$. This second case should be experimentally distinguishable.

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## Table 4

### p-Wave Phase Shifts.

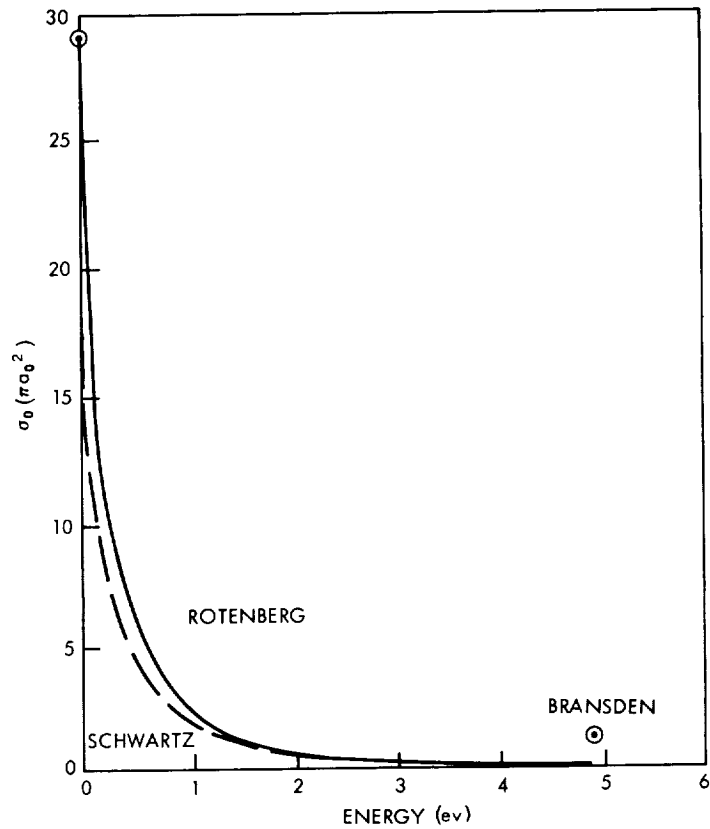| k (ryd $^{1/2}$) | Phase Shift (radians) | |
|---|---|---|
| | Nonadiabatic | Reference 12 |
| 0.1 | 0.00219 | |
| 0.2 | 0.00931 | 0.016 |
| 0.3 | 0.0181 | |
| 0.4 | 0.0277 | 0.104 |
| 0.5 | 0.0371 | |
| 0.6 | 0.04565 | 0.167 |
| 0.7 | 0.0531 | |

## ACKNOWLEDGMENTS

Figure 4—The s-wave scattering cross section of positrons by hydrogen in two approximations. The nonadiabatic p-wave contribution is negligible on this scale whereas Bransden's p-wave (indicated by the point at 5 ev) is not.

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## Appendix A

## List of Symbols

$P_l \left( \cos \theta_{12} \right)$  Legendre polynomials of order $l$ of $\cos \theta_{12}$.

$r_1$  The distance of positron from the nucleus.

$r_2$  The distance of electron from the nucleus.

$R_{ns} \left( r_2 \right)$  The s-eigenstates of hydrogen; in particular $R_{1s} \left( r_2 \right) = 2 r_2^{-r_2}$ is the ground state.

$\delta$  Exact s-wave phase shift.

$\delta_0$  Phase shift of the zeroth order problem; that is,

$$\lim_{r_1 \to \infty} \Phi_0^{(0)} \left( r_1, r_2 \right) = \sin \left( k r_1 + \delta_0 \right) R_{1s} \left( r_2 \right)$$

$\theta_{12}$  The angle between the lines connecting electron and positron to the nucleus.

$\Phi_l \left( r_1 r_2 \right)$  Functions in the basic expansion of

$$\Psi \left( r_1, r_2, \theta_{12} \right) = \frac{1}{r_1 r_2} \sum_{l=0}^{\infty} (2l + 1)^{1/2} \Phi_l \left( r_1, r_2 \right) P_l \left( \cos \theta_{12} \right) \quad .$$

$\Psi \left( r_1 r_2 \theta_{12} \right)$  Solution of the s-wave scattering problem.

$S_{no} \left( r_2 \right)$  The Sturmian functions of order $no$.

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